Electrical Conductivity of Nanotwinned Copper Joints: A First-Principles and Boltzmann Transport Study

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Abstract

Nano-twinned copper is renowned for its outstanding mechanical properties, which enhances mechanical durability while preserving high electrical conductivity and good ductility. High-oriented (111) nano-twinned copper, exhibiting good thermal stability, out-performing oxidation resistance, and excellent resistance to Kirkendall void formation, has emerged as an important material in the packaging field. In this work, we systematically provide the theoretical support for the experimental findings that revealing the highest interface conductivity on (111)-oriented nano-twinned copper joints at 300K through density functional theory (DFT) combined with semiclassical transport theory calculation. By examining various combinations of the crystal directions, we derived the order of conductivity for each interface models. Our results show that Cu<110>/Cu<100> interface exhibits the highest interface conductivity, followed by Cu<111>/Cu<100>, and Cu<111>/Cu<110> interfaces, in decreasing order. On the top of that, our calculations prove that the highest interface conductivity found in experiments can be explained through theoretical calculation and provided the possible combination of varied crystal directions for the bonding joints design.

Keywords - Density functional theory, Semiclassical transport theory, Electrical conductivity, (111)-oriented nano-twinned copper